2,2'-Dihydroxybenzophenone 835-11-0 | DTXSID8022404

Model Performance

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Model	II)ata
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Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.72	51.8	0.74	50.3	0.73	52.7	

Model Results

Predicted value: 80.3 °C

Global applicability domain: Inside

Local applicability domain index: 5.88e-01

Confidence level: 5.20e-01

Nearest Neighbors from the Training Set

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2,2'-Dihydroxybenzophenone

Measured: 59.5 Predicted: 80.3

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Cotoin

Measured: 131 Predicted: 119

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2,2'-Dihydroxy-4-

methoxy benzophen one

Measured: 68.0 Predicted: 99.2

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2,4-Dihydroxybenzophenone

Measured: 144 Predicted: 142

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6-Ethylnaphthalene-2,3-diol

Measured: 149 Predicted: 145